Vinícius Wilian D. Cruzeiro

Postdoctoral researcher, Computational Chemist
Department of Chemistry
SLAC National Accelerator Laboratory
PULSE Institute for Ultrafast Energy Sciences
Stanford University
E-mail: vwcruz@stanford.edu

EDUCATION

UNIVERSITY OF FLORIDA Gainesville, FL, USA
Doctoral degree in chemistry 2014 - 2019
Research: Efficient constant pH and redox potential molecular dynamics with multidimensional replica exchange simulations
Advisor: Dr. Adrian Roitberg
GPA: 4.0/4.0

UNIVERSITY OF SAO PAULO São Paulo, SP, Brazil
Master's degree in physics 2012 - 2014
Research: Thermal effects on the gas-phase absorption spectrum of photosynthetic pigments using classical and *ab initio* molecular dynamics
Advisor: Dr. Kaline Coutinho
GPA: 4.0/4.0

FEDERAL UNIVERSITY OF GOIAS Goiânia, GO, Brazil
Bachelor's degree in physics 2008 - 2011
Research: Applying the electrostatically embedded many-body expansion for faster and accurate *ab initio* molecular dynamics
Advisor: Dr. Herbert Georg
GPA: 4.0/4.0

ACADEMIC EMPLOYMENT

STANFORD UNIVERSITY Stanford, CA, USA
Postdoctoral researcher 2021 – Current
Advisor: Dr. Todd Martinez

UNIVERSITY OF CALIFORNIA, SAN DIEGO San Diego, CA, USA
Postdoctoral researcher 2019 – 2021
Research: 1) Theoretical description of the spectral splitting in the x-ray emission spectrum of liquid water; 2) Developing highly accurate many-body potentials for molecular simulations in atmospheric chemistry; 3) Assessing many-body effects in neural network models
Advisors: Dr. Francesco Paesani and Dr. Andreas Götz

AWARDS AND HONORS (‡ Top 3 awards)

1) *NextProf Science*, University of Michigan (2021). Description: Workshop prepares selected advanced doctoral students and postdoctoral trainees for future faculty career. Program connects people committed to diversity with faculty and academic leaders at the University of Michigan.

2) *Building Future Faculty Program*, North Carolina State University (2020). Description: Granted to a select number of graduate students and post-doctoral scholars who are interested in pursuing academic careers and who are committed to promoting diversity in higher education.

3) ‡ *NVIDIA GPU award*, American Chemical Society (2019). Description: National award given to one researcher who presents work at the COMP session of the ACS national meeting and demonstrates outstanding computational chemistry research carried-out using GPUs, like programming new GPU-

accelerated algorithms or performing simulations with a GPU-accelerated software application; the winner receives a NVIDIA GTX Titan X card.

4) *MolSSI travel award*, The Molecular Sciences Software Institute (2019). Description: Granted to a select number of Ph.D. students and post-doctoral scholars residing in the U.S. the financial support to participate in the 12th European Conference on Computational Theoretical Chemistry and the Open Molecular Science Cloud workshop that was held in Perugia and Rome, Italy; this award supported costs with airfare, registration fee, accommodation, and meals.

5) ‡ *Chemical Computing Group excellence award for graduate students*, American Chemical Society (2018). Description: National award given to graduate students who present work within the COMP program at the ACS national meeting; this award includes a stipend to cover travel expenses and an honor ceremony.

6) *Early career physical chemistry award*, University of Florida (2015). Description: Given to the top overall performing first-year graduate student in physical chemistry.

7) ‡ *Townes R. Leigh award*, University of Florida (2015). Description: Given for outstanding achievement by first-year graduate students. This award recognizes excellence in coursework, teaching, research, and written qualifying examinations.

8) *Grinter fellowship*, University of Florida (2014). Description: Awarded to outstanding prospective students as a recruitment incentive.

9) *Graduate fellowship* for studies at the University of Florida, CAPES, Brazil (2014-2018). Description: Awarded to outstanding students that desire to obtain a doctoral degree abroad. This fellowship is part of the *Science without borders* program.

10) *Graduate fellowship* for studies at the University of São Paulo, CNPq, Brazil (2012-2014). Description: Awarded to the top-ranked students in the admission selection process.

11) *Undergraduate research scholarship*, CNPq, Brazil (2009-2011). Description: Awarded to encourage undergraduate students with outstanding academic records to have their first contact with scientific research.

PUBLICATIONS

1) **Cruzeiro, V.W.D.;** Wildman, A.; Li, X.; Paesani, F.; On the relationship between hydrogen-bonding motifs and the $1b_1$ splitting in the x-ray emission spectrum of liquid water. *J. Phys. Chem. Lett.*, 12: 3996 (2021).

2) **Cruzeiro, V.W.D.;** Lambros, E.; Riera, M.; Roy, R.; Paesani, F.; Götz, A.; Highly accurate many-body potentials for simulations of N_2O_5 in water: benchmarks, development, and validation. *J. Chem. Theory Comput.*, 17: 3931 (2021). (• *Front cover of the journal)*

3) **Cruzeiro, V.W.D.;** Manathunga, M.; Merz, K.M.; Götz, A.; Open-Source Multi-GPU-Accelerated QM/MM Simulations with AMBER and QUICK. *J. Chem. Inf. Model*, 61: 2019 (2021). *(• Highlighted with a press release)*

4) Manathunga, M.; Jin, C.; **Cruzeiro, V.W.D.;** Miao, Y.; Mu, D.; Arumugam, K.; Keipert, K.; Aktulga, H.M.; Merz, K.M.; Götz, A.; Harnessing the Power of Multi-GPU Acceleration into the Quantum Interaction Computational Kernel Program. *J. Chem. Theory Comput.*, ACCEPTED (2021). *(• Highlighted with a press release)*

5) Bueno, P.; **Cruzeiro, V.W.D.;** Roitberg, A.; Feliciano, G.; The density-of-states and equilibrium charge dynamics of redox-active switches. *Electrochim. Acta*, 387: 138410 (2021).

6) **Cruzeiro, V.W.D.;** Feliciano, G.T.; Roitberg, A.E.; Exploring coupled redox and pH processes with computational chemistry: applications to five different systems. *J. Am. Chem. Soc.*, 142: 3823 (2020). *(• Highlighted in JACS Spotlights)*

7) **Cruzeiro, V.W.D.;** Gao, X.; Kleiman, V.D.; Implementing new educational platforms in the classroom: an interactive approach to the particle in a box problem. *J. Chem. Educ.*, 96: 1663 (2019).

8) **Cruzeiro, V.W.D.;** Roitberg, A.E.; Multidimensional replica exchange simulations for efficient constant pH and redox potential molecular dynamics. *J. Chem. Theory Comput.*, 15: 871 (2019).

9) **Cruzeiro, V.W.D.;** Amaral, M.S.; Roitberg, A.E.; Redox potential replica exchange molecular dynamics at constant pH in Amber: Implementation and validation. *J. Chem. Phys.*, 149: 072338 (2018). *(• Front cover of the journal. • 2018 JCP Editors' Choice article. • Featured paper. • Highlighted with a press release)*

10) Bell, M.R.; **Cruzeiro, V.W.D.;** Cismesia, A.P.; Tesler, L.F.; Roitberg, A.E.; Polfer, N.C.; Probing the structures of solvent-complexed ions formed in electrospray ionization using cryogenic infrared photodissociation spectroscopy. *J. Phys. Chem. A*, 122: 7427 (2018).

11) Chouinard, C.D.; **Cruzeiro, V.W.D.;** Kemperman, R.H.J; Oranzi, N.R.; Roitberg, A.E.; Yost, R.A.; Cation-dependent conformations in 25-hydroxyvitamin D3-cation adducts measured by ion mobility-mass spectrometry and theoretical modeling. *Inter. J. Mass Spectrom.*, 432: 1 (2018).

12) Chouinard, C.D.; **Cruzeiro, V.W.D.;** Roitberg, A.E.; Yost, R.A.; Experimental and theoretical investigation of sodiated multimers of steroid epimers with ion mobility-mass spectrometry. *J. Am. Soc. Mass Spectrom.*, 28: 323 (2017).

13) Chouinard, C.D.; **Cruzeiro, V.W.D.;** Beekman, C.R.; Roitberg, A.E.; Yost, R.A.; Investigating differences in gas-phase conformations of 25-hydroxyvitamin D3 sodiated epimers using ion mobility-mass spectrometry and theoretical modeling. *J. Am. Soc. Mass Spectrom.*, 28: 1497 (2017).

14) **Cruzeiro, V.W.D.;** Roitberg, A.E.; Polfer, N.C.; Interactively Applying the variational method to the dihydrogen molecule: exploring bonding and antibonding. *J. Chem. Educ.*, 93: 1578 (2016).

15) Bhatt, A.; Mahon, B.P.; **Cruzeiro, V.W.D.;** Cornelio, B.; Laronze-Cochard, M.; Ceruso, M.; Sapi, J.; Rance, G.A.; Khlobystov, A.N.; Fontana, A.; Roitberg, A.; Supuran, C.T.; McKenna, R.; Structure activity relationships of benzenesulfonamide-based inhibitors towards carbonic anhydrase isoform specificity. *Chembiochem*, 18: 213 (2016).

16) Cabral, B.J.C.; **Cruzeiro, V.W.D.;** Coutinho, K.; Canuto, S; Free base phthalocyanine: influence of thermal effects and dimerization on the electronic absorption spectrum. *Chem. Phys. Let.*, 595: 97 (2014).

PUBLICATIONS IN REVIEW

17) **Cruzeiro, V.W.D.;** Lambros, E.; Riera, M.; Roy, R.; Paesani, F.; Götz, A.; Insights into the uptake of N_2O_5 by aqueous aerosol using chemically accurate many-body potentials. *J. Phys. Chem. Lett.* (2021). (*Available in ChemRxiv*)

18) Ahn, S.; Seitz, C.; **Cruzeiro, V.W.D.;** McCammon, J.A.; Götz, A.; Data for molecular dynamics simulations of escherichia coli cytochrome bd oxidase with the amber force field. *Data Brief* (2021). (*Available in ChemRxiv*)

RESEARCH EXPERIENCE

UNIVERSITY OF CALIFORNIA, SAN DIEGO, Postdoctoral research San Diego, CA, USA
Advisor: Dr. Francesco Paesani 2019 - 2021

Main project:

- Investigated the x-ray emission spectrum of liquid water that exhibits a spectral split in the $1b_1$ region associated with the hydrogen-bonding environment. Despite previous theoretical and experimental research on this feature, the hydrogen-bonding motifs that give rise to the splitting were not yet described.
- Made use of path integral molecular dynamics (PIMD) with the MB-pol model. These simulations accurately describe water across different phases and contain quantum nuclei effects.
- Performed TD-DFT calculations aiming at high-energy emissions for the study of the split spectral feature.
- Provided novel insights from a theoretical perspective about the different hypotheses in the literature that attempt to describe the origin of this spectrum feature. Showed the relation between the different hydrogen-bonding motifs and the theoretical x-ray emission spectrum.
- Computed the spectrum at different temperatures and observed trends for the relative intensity of the two peaks in the $1b_1$ region that are in good agreement with experimental observations.

Other contributions:

- Explored how many-body effects are described in deep neural networks.

Advisor: Dr. Andreas Götz 2019 - 2021

Main project:

- Employed accurate fitting approaches and fragmentation methods to generate potentials with CCSD(T) accuracy for molecular simulations of clusters, interfaces, and bulk.
- The new potentials follow the same characteristics of the highly successful MB-pol water model, which combines a physically motivated representation of long-range interactions with accurate low-order terms of the many-body expansion. MB-pol accurately describes experimental properties of water across different phases.
- Newly generated potentials were used in simulations of dinitrogen pentoxide (N_2O_5) in water, which are relevant in atmospheric chemistry because N_2O_5 is an important intermediate in reactions of nitrogen oxides related to air quality and climate. This project was part of the Center for Aerosol Impacts on Chemistry of the Environment (CAICE), an NSF funded institution with 26 experimental and theoretical groups.

Other contributions:

- Implemented in Sander (MD engine from Amber) an interface to the *ab initio* quantum chemistry software Quick which allows QM/MM simulations with multi-GPU-acceleration. Since Quick and Sander are open source, these simulations can be performed free of charge.
- Computed Amber force field parameters for heme b_{558}, heme b_{595}, and heme d, enabling simulations of *Escherichia coli* cytochrome *bd* oxidase and related systems.

UNIVERSITY OF FLORIDA, Doctoral degree in chemistry Gainesville, FL, USA
Advisor: Dr. Adrian Roitberg 2014 - 2019

Main project:

- Developed, tested, validated, and implemented in Amber new methods that allow the theoretical study of electrochemical processes through simulations at constant redox potential and pH.
- Implemented in Amber new replica exchange techniques that allow converged results to be obtained more efficiently.
- All these new Amber implementations are available using GPU-accelerated code, which provides high-performance to the simulations. These are the first implementations of constant redox potential methods in a common molecular dynamics package.

Other contributions:

- Collaborated with different experimental groups by applying computational chemistry to aid in explaining a variety of problems, like different epimer conformers in Ion Mobility-Mass Spectrometry experiments, inhibitor functionality in cancer drug targets, and conformations of solvent-tagged ions in infrared photodissociation spectroscopy experiments.

UNIVERSITY OF SAO PAULO, Master's degree in physics São Paulo, SP, Brazil
Advisor: Dr. Kaline Coutinho 2012 - 2014

- Studied thermal effects on the gas-phase electronic absorption spectrum of monomers and dimers of different porphyrins and phthalocyanines. Classical and *ab initio* molecular dynamics were employed.
- Proposed a new set of force field parameters to reproduce better the conformations yielded by *ab initio* molecular dynamics.
- Performed experimental measures of the absorption spectra of phthalocyanines as a function of pH.

FEDERAL UNIVERSITY OF GOIAS, Bachelor's degree in physics Goiânia, GO, Brazil
Advisor: Dr. Herbert Georg 2009 - 2011

- Applied the many-body expansion as an approach to significantly speedup *ab initio* molecular dynamics simulations without meaningful loss in accuracy. This methodology has been employed to reproduce post-HF calculations.
- Implemented a software to perform many-body expansion and molecular dynamics calculations. Electronic structure calculations are performed on an external software.

MOST RELEVANT CONFERENCE PRESENTATIONS (Out of a total of 28)

Cruzeiro, V.W.D.; Paesani, F.; Theoretical description of the $1b_1$ splitting in the x-ray emission spectrum of liquid water. **Oral presentation;** Virtual Conference in Theoretical Chemistry, Online, Stanford University (2020). (• *Presented as a featured speaker for winning Outstanding Lightning Talk competition*)

Cruzeiro, V.W.D.; Possible applications for the open molecular science cloud: Amber simulations and development of highly accurate many-body potentials. **Oral presentation;** 12th European Conference on Computational and Theoretical Chemistry, Perugia and Rome, Italy (2019).

Cruzeiro, V.W.D.; Roitberg, A.E.; GPU-accelerated constant pH and redox potential molecular dynamics: exploring electrochemistry in Amber. **Sci-Mix and COMP poster presentation;** 257th ACS National Meeting and Exposition, San Diego, CA, USA (2019).

Cruzeiro, V.W.D.; Roitberg, A.E.; Efficient constant pH and redox potential molecular dynamics with multidimensional replica exchange simulations. **Sci-Mix and COMP poster presentation;** 256th ACS National Meeting and Exposition, Boston, MA, USA (2018).

Cruzeiro, V.W.D.; Roitberg, A.E.; High-performance multidimensional replica exchange molecular dynamics along pH, redox potential and temperature dimensions using Amber. **Sci-Mix and COMP poster presentation;** 255th ACS National Meeting and Exposition, New Orleans, LA, USA (2018).

Cruzeiro, V.W.D.; Roitberg, A.E.; Applying theoretical modeling to help the interpretation of ion mobility/mass spectrometry experiments: the case of cation-dependent 25-hydroxyvitamin D3 conformations. **Oral and poster presentation;** ASMS Sanibel Conference, St. Petersburg, FL, USA (2018).

Cruzeiro, V.W.D.; Amaral, M.S.; Roitberg, A.E.; High-performance molecular dynamics at constant pH and constant redox potential using Amber. **Oral presentation;** 253rd ACS National Meeting and Exposition, San Francisco, CA, USA (2017).

Cruzeiro, V.W.D.; Roitberg, A.E.; Applying theoretical modeling to help the interpretation of ion mobility/mass spectrometry experiments. **Oral presentation;** 91st Florida Annual Meeting and Exposition (FAME), Tampa, FL, USA (2016).

Cruzeiro, V.W.D.; Georg, H.C.; Applying the many-body expansion for *ab initio* molecular dynamics. **Oral presentation;** II Brazilian School of Molecular Modeling, Santo André, Brazil (2013).

Cruzeiro, V.W.D.; Coutinho, K.; Cabral, B.J.C.; Canuto, S.; Theoretical study of the absorption spectra of photosynthetic pigments. **Poster presentation;** Workshop on Biomolecular Theory-Experiment Interplay, São Paulo, Brazil (2013).

COMPUTATIONAL SKILLS

Languages: Fortran, Python, Bash, C++, CUDA, MPI, OpenMP, PHP, HTML, SQL.
Experience: Amber developer (since 2017), parallel programming, object-oriented programming, server management, web developer.
Contributions to Amber (popular software for molecular simulations): 1) Constant pH and redox potential molecular dynamics in both implicit and explicit solvent; 2) Redox potential replica exchange molecular dynamics; 3) Multi-dimensional replica exchange support for pH and redox potential dimensions; 4) Implemented an interface with Quick that allows multi-GPU-accelerated QM/MM simulations; 5) Implementation of new AmberTools for preparation of input files and analyses of output files; 6) Several bug fixes.

TEACHING EXPERIENCE

UNIVERSITY OF FLORIDA Gainesville, FL, USA
Graduate Teaching Assistant 2014 – 2019

- Development of educational interactive platforms that allow students to better explore the class material. (See publications in the *J. Chem. Educ.*)
- Graduate courses taught:
    - CHM6586 - Computational Chemistry. Description: this course is offered to students from different departments that have different backgrounds. The students gain practical experience (on how to choose a good combination of method/basis set, how to perform basis set extrapolation, etc.) as well as a theoretical basis behind common algorithms (as self-consistent field, geometry optimization, and frequency calculations) and methods (like Hartree-Fock, MP2, and DFT) in electronic structure software.
    - CHM6470 - Chemical Bond & Spectra 1. Description: in this course, students learn quantum mechanics, with a focus in theoretical chemistry.
- Undergraduate courses taught:
    - CHM4411 - Physical Chemistry
    - CHM3400 - Physical Chemistry with Applications to Biology

UNIVERSITY OF SAO PAULO São Paulo, SP, Brazil
Teaching Assistant 2012 – 2014

- Undergraduate courses taught:
    - Physics I
    - Introduction to Physics

FEDERAL UNIVERSITY OF GOIAS Goiânia, GO, Brazil
Teaching Assistant 2009 – 2011

- Undergraduate courses taught:
    - Physics I
    - Physics II

VOLUNTEER EXPERIENCE

Letters to a Pre-Scientist
Role: Scientist Pen Pal Aug. 2018 – Current

- This program connects students from high-poverty schools with real scientists. The idea is that this connection can help with students' education. From this "scientific interaction", that most students likely would not have otherwise, they may be encouraged to afterwards follow a STEM career.

ASSOCIATIONS

Member of the *American Chemical Society*.

Member of the *Brazilian Physical Society*.

REFERENCES

Dr. Todd Martinez
Department of Chemistry
Stanford University
333 Campus Drive
Stanford, CA 94305
E-mail: todd.martinez@stanford.edu

Dr. Francesco Paesani
Department of Chemistry and Biochemistry
University of California, San Diego
6218 Urey Hall
La Jolla, CA 92093
E-mail: fpaesani@ucsd.edu

Dr. Adrian Roitberg
Department of Chemistry
University of Florida
440 Leigh Hall
Gainesville, FL 32611
E-mail: roitberg@ufl.edu

Dr. Andreas Götz
San Diego Supercomputer Center
University of California, San Diego
10100 Hopkins Dr.
La Jolla, CA 92093
E-mail: agoetz@sdsc.edu

Dr. Rodney Bartlett
Department of Physics
University of Florida
Quantum Theory Project
2338 New Physics Building
PO Box 118435
Gainesville, FL 32611
E-mail: bartlett@qtp.ufl.edu

Dr. Kaline Coutinho
Department of Physics
University of São Paulo
Rua do Matão, nº 1371
Ed. Principal - Ala 2, Sala 207
São Paulo, Brazil, 05508-090
E-mail: kaline@if.usp.br